

1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-
376-18-1 | DTXSID3059923

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.72e-02 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.67e-01

Confidence level: 2.52e-01

Nearest Neighbors from the Training Set

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1,2-Dichloro-4-(trifluoromethyl)benzene

Measured: 5.25e-01

Predicted: 2.42

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2-Butene, 1,1,1,2,3,4,4,4-octafluoro-

Measured: 1.33e-01

Predicted: 2800

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Benazolin

Measured: 4.28e-07

Predicted: 8.30e-09

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Silane, chlorodimethylphenyl-

Measured: 2.91

Predicted: 1.01

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Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-

Measured: 33.1

Predicted: 2170